

the Analytical Scientist

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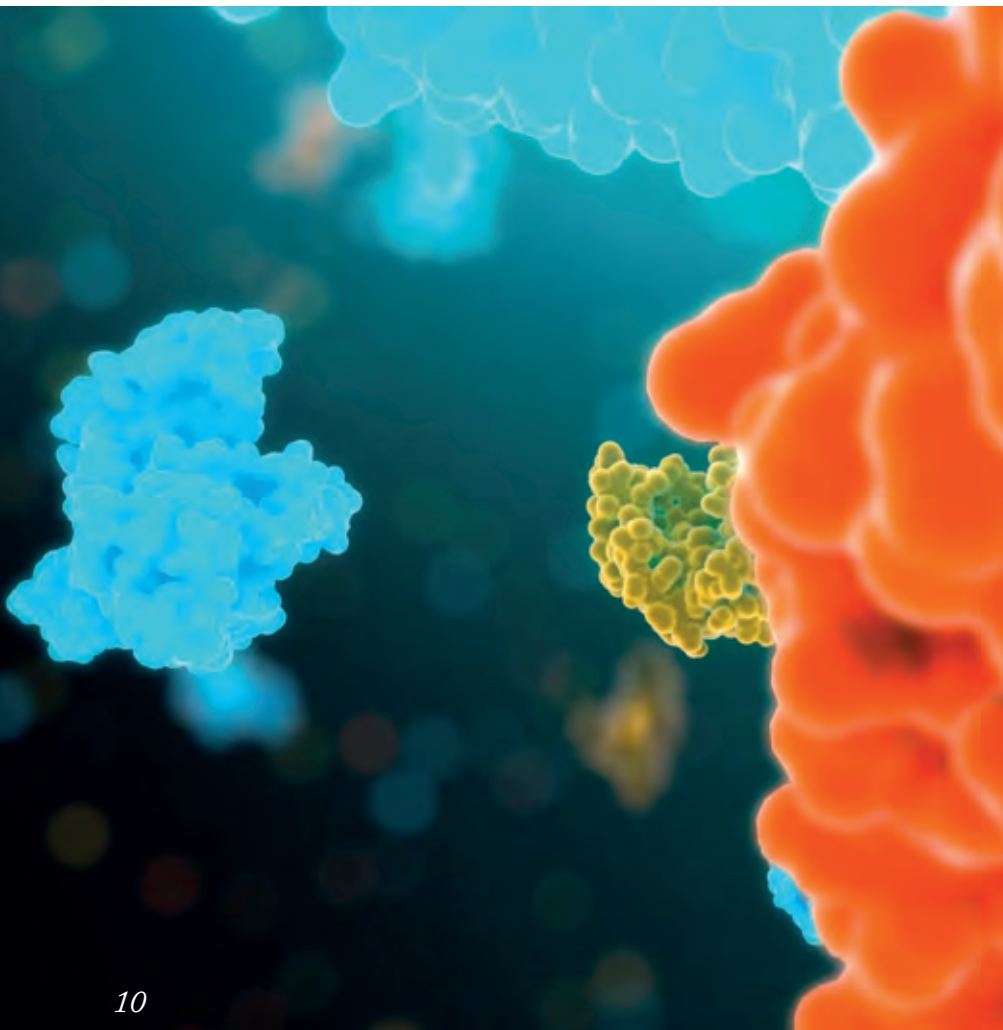
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**Editor** - Rich Whitworth

rich.whitworth@texerepublishing.com

Associate Editor - Joanna Cummings

joanna.cummings@texerepublishing.com

Scientific Director - Frank van Geel

frank.vangeel@texerepublishing.com

Editorial Director - Fedra Pavlou

fedra.pavlou@texerepublishing.com

Publishing Director - Lee Noyes

lee.noyes@texerepublishing.com

Sales Manager - Chris Joinson

chris.joinson@texerepublishing.com

Senior Designer - Marc Bird

marc.bird@texerepublishing.com

Designer - Emily Strefford-Johnson

emily.johnson@texerepublishing.com

Digital Content Manager - David Roberts

david.roberts@texerepublishing.com

Mac Operator Web/Print - Peter Bartley

peter.bartley@texerepublishing.com

Tablet Producer - Abygail Bradley

abygail.bradley@texerepublishing.com

Audience Insight Manager - Tracey Nicholls

tracey.nicholls@texerepublishing.com

Traffic and Audience Associate - Lindsey Vickers

lindsey.vickers@texerepublishing.com

Traffic and Audience Associate - Jody Fryett

jody.fryett@texerepublishing.com

Apprentice, Social Media / Analytics - Ben Holah

ben.holah@texerepublishing.com

Events and Office Administrator

- Alice Daniels-Wright

alice.danielswright@texerepublishing.com

Financial Controller - Phil Dale

phil.dale@texerepublishing.com

Chief Executive Officer - Andy Davies

andy.davies@texerepublishing.com

Chief Operating Officer - Tracey Peers

tracey.peers@texerepublishing.com

Editorial Advisory BoardMonika Dittmann, *Agilent Technologies, Germany*Norman Dovichi, *University of Notre Dame, USA*Gary Hietje, *Indiana University, USA*Emily Hilder, *University of Tasmania, Australia*Ron Heeren, *FOM-AMOLF, The Netherlands*

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tracey.nicholls@texerepublishing.com

Tracey Nicholls, The Analytical Scientist,

Texere Publishing Ltd, Haig House, Haig Road,

Knutsford, Cheshire, WA16 8DX, UK

General enquiries:

www.texerepublishing.com

info@texerepublishing.com

+44 (0) 1565 745200

sales@texerepublishing.com

Distribution:

The Analytical Scientist (ISSN 2051-4077),

is published monthly by Texere Publishing

Ltd and is distributed in the USA by UKP

Worldwide, 1637 Stelton Road B2,

Piscataway, NJ 08854.

Periodicals Postage Paid at Piscataway,

NJ and additional mailing offices

POSTMASTER: Send US address changes to

The Analytical Scientist, Texere Publishing Ltd,

C/o 1637 Stelton Road B2,

Piscataway NJ 08854

Single copy sales £15 (plus postage, cost available

on request tracey.nicholls@texerepublishing.com)

Annual subscription for non-qualified recipients £110

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On The Cover

*Women get vocal about
(in)equality. Pastiche
of Franz Ferdinand's
album "You Could Have
It So Much Better" (itself
a pastiche of Rodchenko's
iconic constructivist poster).***Upfront**

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- 50 **Chris Pohl**, Vice President, Chromatography Chemistry, Thermo Fisher Scientific, San Francisco Bay Area, USA.

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systems can run 24/7 without human intervention, such 'smart' automated systems can facilitate high sample throughput, allowing scientists to focus on the skilled analysis and interpretation of the results rather than on time-consuming wet chemistry or sample injection.

For example, we recently worked on a metabolomics study of algae cell cultures using a PAL RTC platform, which involved a pretty complex pre-analytical process (3). We combined Bligh and Dyer (LLE) extraction with dual-column UHPLC-MS/MS separation and detection in an automated setup (which included adding the set reagents and splitting the aqueous and organic fractions prior to injection into the UHPLC system). Even with an initial manual step, the automated method proved significantly less labor-intensive than the manual technique and also allowed the results to be directly subjected to a library search using LC-MS/MS data in SWATH mode (SCIEX), meaning that further targeted experiments to

identify unknowns were unnecessary. Moreover, when compared with the manual method, the automated setup had better repeatability for both aqueous and organic fractions.

Analytical scientists, regardless of industry or sector, are all aiming towards a common goal: achieving the best quality results as efficiently as possible. Taking a smart approach to automating the sample preparation process cuts the 'garbage' being fed into the sample analysis process and improves data quality and speed of delivery to researchers – and thereby reduces the 'garbage' output from the lab.

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On the -Omics Journey

**Profiling and fingerprinting
in food analysis signposts a
route to a better life.**



*By Chiara Cordero, Associate Professor
of Food Chemistry, Department of Drug
Science and Technology, University of
Turin, Italy.*

Modern '-omics' disciplines applied to food (foodomics, sensomics) focus analytical efforts on elucidating bioactive compounds (nutrients and non-nutrients, active secondary metabolites, pre-biotics, odorants and tastants) – essentially, all possible chemical stimuli for food-body interactions (1–3). The ultimate aim is to understand the intriguing – though rather complex – crosstalk between 'what we eat and why, and what we are'. Such investigation requires a comprehensive and integrated approach that will detail a food sample's constituents, in terms of physicochemical properties, concentration in the matrix, distribution throughout the body and, within the "-omics" concept, the physiological activity or sensory properties (odor/taste quality, perception threshold). These comprehensive analyses require multidimensional and hyphenated

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analytical platforms capable of exploring all the chemical information dimensions with a detailed profiling approach (4, 5) and all the inter-connecting sample information dimensions (for example, those related to the biological phenomenon being studied) using advanced fingerprinting techniques (6, 7).

‘What we eat’ is one side of the coin that we need to understand in (chemical) detail so that we know the exact composition to i) differentiate high quality from mass produced products, ii) enable the authentication of a specific botanical/geographical origin or iii) assist technologists during industrial processing with a view to defining a quality benchmark. ‘What we are’ relates mainly to the interaction of food components within our body. It goes beyond the nutrition domain and includes the effect of non-nutrients and bioactive compounds that may promote health and wellness (nutraceuticals).

Over the last ten years, our research group has dedicated a lot of effort to exploring these concepts and implementing “simple” comprehensive two-dimensional gas chromatographic (GC×GC) platforms and further orthogonal dimensions, including mass spectrometry (MS), olfactometry, automated sample preparation and advanced data mining (8–10). The latter hyphenation, which is fundamental when exploring and interpreting complex data, was realized

thanks to the collaboration with experts in other fields. Stephen Reichenbach (Computer Science & Engineering Dept., University of Nebraska–Lincoln, USA) has taken on this challenge and has developed intuitive, effective software solutions for 2D data mining.

Thanks to the superior informing power of GC×GC-MS, we have studied complex fractions of volatiles from high-quality hazelnuts, raw and roasted coffee, green and black tea, dried milk, plant extracts and essential oils. Every analytical run provides a deep insight into the chemical complexity of each sample and provides new perspectives in food chemical investigations that, just a decade ago, were inconceivable – or at least not possible without laborious and time-consuming pre-concentration steps. Looking at the food component distribution and interaction with the body, metabolomics is encouraging collaborative and fascinating studies on the effects of diet and physical exercise on Type 2 diabetes in mice models and in humans (11, 12).

The multi-multi dimensional platforms we have experimented with, thanks to the inspiration of our “boss” (Carlo Bicchi) and the creativity of new generations of scientists, have both intrigued industry and initiated further collaboration. The primary objective? To transfer new concepts in chemical measurements to ‘real-world’ applications. The vision? To see –omics

concepts applied to routine analysis. I believe this will enable quality food chemical characterization, by-product valorization, and bioactive compounds profile activity to be controlled and monitored – all of which will have a positive effect on our lives and society. To that end, academic research must take advantage of the support made available by instrument companies to help direct research effectively through prototyping new analytical solutions for QA and QC laboratories. For example, our collaboration with Agilent and SRA Instruments (Italy) enabled us to transfer most of the “-omics” applications developed for thermal modulated GC×GC-MS platforms to the simpler and cost effective differential flow modulated systems (13–16). Those of you at Riva 2016 will have (had) the chance to see me deliver this work in person (tas.txp.to/0516/riva2016). A prototype is now ready to launch and we are all looking forward to where it will take us on our –omics journey!

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- 1–15 Available only online: tas.txp.to/0516/Cordero
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Two Words: Food Scanners

H2020 wanted to put food authentication into the hands of the consumer. What impact will the outcome have on our field?



By Yannick Weese, researcher, Authenticity and Nutrients Business Unit, RIKILT Wageningen UR, The Netherlands.

Two years ago (in June 2014) and by mere coincidence, I entered the field of

vibrational spectroscopy. I was starting my first ‘real’ job as a young researcher at RIKILT in Wageningen. My business unit deals with food authenticity and fraud, multivariate statistics, analytical techniques and many different food types. We looked at what we were doing in the lab and reassigned the tasks, and then I found myself leading the near-infrared, mid-infrared, and Raman spectroscopy division. At that point, I hadn’t fully appreciated the revolution going on in the